

# Industry Application



## A Forensic Database Administered by RTI International

RTI International is one of the world's leading research institutes, dedicated to improving the human condition by turning knowledge into practice by providing research and technical expertise to governments and businesses in more than 40 countries. As part of an effort to strengthen the scientific basis for forensics toxicology and drug testing, RTI, with a grant from the National Institute of Justice, sought to create a database of spectral and chemical information on toxins, pharmaceuticals, and illicit substances of relevance to the forensic community. The question became how to create and manage a database that could be accessible to the public, and could be built from data acquired by users and laboratories around the world?

The solution was analytical data handling and databasing software from ACD/Labs enabling the creation of the 'Forensic DB' ([www.forensicdb.org](http://www.forensicdb.org)), a web-based cheminformatics database for the retention, review, and ongoing collection of spectral data pertaining to toxins, drugs, and other compounds of interest to the forensics community.

ACD/Labs software allows for the creation of relational databases of analytical spectra, data, chemical structures, and properties with powerful searching capabilities and accessibility features. A web-enabled searching and browsing tool requires only an internet connection for users to be able to access database content, while maintaining security through a login and authentication system. These features made the software well suited to RTI's vision for the Forensic DB.

Originally the goal for the Forensic DB was to house GC/MS and Direct Analysis in Real-Time (DART) MS spectra and associated data, however, the capability also exists for future expansion to include LC/MS, UV and Raman Data, and even NMR data in the future. As part of the project, ACD/Labs developed a peer-review data submission system which allows the Forensic DB to accept analytical data submitted by users, storing it in a temporary database, pending approval by collaborators, for inclusion into the Forensic DB.

Currently, all database records include compound structure, data regarding the source and collection information, and the spectra included as searchable data, rather than simply as an image. IUPAC nomenclature and various relevant physicochemical properties, such as  $pK_a$ , are predicted and added to new records. Users can upload spectra to search for matching examples, perform structure and substructure queries, as well as generate reports.

As the number of contributing users to the Forensic DB grows, the database will become a comprehensive compendium of toxins, pharmaceuticals, and illicit substances for use by forensic laboratories, researchers, and law enforcement. The Forensic DB web site also includes a discussion forum for users and information on submitting analytical data for review.

*"ACD/Labs provided the tools necessary to host the data and manage a system wherein new data will be peer reviewed before it is made public. It has expanded the scope and functionality of the original project significantly."*

Peter Stout,  
Curator Forensic DB and Senior Forensic  
Research Toxicologist at RTI International

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